# Two Multi-setting Causal Inequalities and Their Violations

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In this paper, two simple causal inequalities with 4 inputs and 2 outputs are derived. To this end, we have introduced two causal games, and the corresponding inequality can be derived as an upper bound of the success probability under the causal order. Those inequalities can be violated by choosing proper process matrices and instruments. Moreover, the violation for one of them is maximal when the instruments are restricted to be binary ones.

### 1. INTRODUCTION

One of remarkable features of quantum mechanics is that it violates the local realism, namely, the observable physical quantity has uncertainty before being measured [1]. Thanks to the famous Bell theorem, which shows that the non-locality is an intrinsic property of quantum theory [2]. It is noticeable that the correlations involved in those works are no-signaling ones. This means that the observers are located in isolate spaces, and the correlations between them can be obtained by measuring a bipartite state. However, we can also consider the signaling correlations. In this case, the observers can communicate with each other through a quantum channel. A concept related to the signaling correlation is causal order, on which a common cognition is that events of the past will affect the future events, but not vice versa. People's intuition is that there are definite causal relations between the past events and the future ones.

However, this point of view is challenged in quantum theory. In 2012, Oreshkov et al. [3] found a new framework called process matrix (see the preliminaries for the definition), which relaxes the assumptions on any definite causal structures of local operations. Assuming all observers admit quantum mechanics (i.e., operations of each party in its closed laboratory can be described by quantum theory), it can be shown that the correlations between them are noncausal and incompatible with any pre-defined causal order, and it violates the bipartite causal inequality, that is the constraints satisfied by correlations generated in any definite causal order. Such a result aroused widespread concern immediately [4-13].

The scenario of the causal model has many analogy to the Bell scenario. For instance, the process matrix is a generalization of quantum states and the instruments are the analogy of the positive operator valued measurements (POVMs). However, the causal scenario is totally different to the Bell scenario, because the causal scenario is based on a signaling correlation while in the Bell scenario, the observers are forbidden to have any communicates. Contrast to the vast literatures about the Bell scenario and Bell inequalities, there are not too much work about causal model and causal inequalities.

In this paper, we will study two causal inequalities which are motived by the inequalities considered in Ref. [3] and Ref. [4]. To this end, we will introduce two causal games. By using all strategies under the causal order, there is an upper bound for the success probability of the corresponding game, which leads to our causal inequality (see inequalities (8) and (9)). Our games involve 4 inputs, which can also be extended to  $2^n$  inputs. The most difficult part of our work is to choose proper process matrix and instruments to violate the inequalities. Moreover, using the method proposed by Brukner [14], the obtained violation for the inequality (9) is proved to be maximal in the sense of restricting the outputs to be binary.

## 2. PRELIMINARIES

**Causal Games.** Let  $\pi$  be a probability distribution on  $A \times B$ , and let V be a predicate on  $X \times Y \times A \times B$ , for sets A, B, X and Y. Then V and  $\pi$  define a game  $G = G(V, \pi)$  as follows. Assume there are two players Alice and Bob against a referee. The referee randomly chooses values  $a \in A, b \in B$  according the the distribution  $\pi$  and sends them to Alice and Bob, respectively. Alice and Bob respond by sending answers  $x \in X$  and  $y \in Y$  to the referee. Not like to the nonlocal game, a causal game allows the players to communicate to each other. They win if V evaluates to 1 on (x, y, a, b) and lose otherwise. We will denote the value of the predicate V on (x, y, a, b) as V(x, y|a, b). The success

probability of a game  $G(V, \pi)$  is defined as follows:

$$p_G := \sum_{x,y,a,b \in (X,Y,A,B)} \pi(a,b) p(x,y|a,b) V(x,y|a,b),$$
(1)

where p(x, y|a, b) is the joint probability of obtaining x, y whenever Alice and Bob receive a and b respectively. Usually the joint probability is used to describe the correlation between the two players.

Strategies under the causal order. If Alice's operations fall behind Bob's (we denote  $B \leq A$ ), then Bob can transmit his information to Alice, but Alice is forbidden to send signal to Bob. In this case, their correlation is denoted by  $p^{B \leq A}(x, y|a, b)$ , which satisfies  $p^{B \leq A}(y|a, b) = p^{B \leq A}(y|a', b), \forall a, a', b, y$ , and  $p^{B \leq A}(y|a, b) = \sum_{x} p^{B \leq A}(x, y|a, b)$ . Similarly, we can define  $p^{A \leq B}(x, y|a, b)$ , etc. A joint probability p(x, y|a, b) is called causal if there is some  $r \in [0, 1]$  such that [5, 6]:

$$p(x, y|a, b) = rp^{B \preceq A}(x, y|a, b) + (1 - r)p^{A \preceq B}(x, y|a, b).$$
(2)

**Examples.** In Ref. [3], Oreshkov et al. introduced a causal game called "guess your neighbor's input by tossing a coin" (GYNIC), namely, one of the player Bob will toss a coin, Alice and Bob's performances are based on the results of the coin. Briefly this game can be described as follows: Alice and Bob receive randomly uniform inputs  $a, b \in \{0, 1\}$  from the referee, respectively. Bob has another bit b'. If b' = 0, Alice need to guess Bob's input bit b. And if b' = 1, Bob need to guess Alice's input bit a. Denote the guessing results of Alice and Bob by  $x, y \in \{0, 1\}$  respectively. GYNIC is defined by letting  $\pi(a, b, b') = \frac{1}{8}$  and

$$V(x, y|a, b, b') = \begin{cases} \delta_{x, b}, & \text{if } b' = 0\\ \delta_{y, a}, & \text{if } b' = 1. \end{cases}$$

It was shown that by using all strategies under the causal order, namely the joint probability p(x, y|a, b, b') satisfies the constraint (2), we have

$$p_{\text{GYNIC}} = \frac{1}{2} p(x = b \mid b' = 0) + \frac{1}{2} p(y = a \mid b' = 1) \le 0.75.$$
(3)

In the casual game GYNIC, the random bit b' controls the game. Different to the game GYNIC, Branciard et al. [4] obtained a simpler game named "guess your neighbor's input" (GYNI) in 2016, in which the additional bits b' are not required. To win the game, Alice (resp. Bob) should guess the response of Bob (resp. Alice) correctly. More precisely, GYNI is defined by letting

$$\begin{cases} \pi(a,b) = \frac{1}{4}, \\ V(x,y|a,b) = \delta_{x,b}\delta_{y,a} \end{cases}$$

where x, y and a, b take values in  $\{0, 1\}$ . By using all causal strategies, the success probability of GYNI is upper bounded by

$$p_{\text{GYNI}} = p(x = b, y = a) \le \frac{1}{2}.$$
 (4)

**Process matrix and instrument.** Let  $H^{A_I}$  and  $H^{B_I}$  be the input Hilbert spaces,  $H^{A_O}$  and  $H^{B_O}$  be the output Hilbert spaces of Alice and Bob, respectively. For simplicity, we denote  $H^X$  by X, and  $H^X \otimes H^Y \otimes H^Z$  by XYZ, etc. An operator  $W \in L(H^{A_I} \otimes H^{A_O} \otimes H^{B_I} \otimes H^{B_O})$  is called process matrix [3] if it satisfies the following conditions [6]:

$$W \ge 0, \text{ Tr}W = d_{A_O}d_{B_O},$$
  

$$B_IB_O W =_{A_OB_IB_O} W, A_IA_O W =_{A_IA_OB_O} W,$$
  

$$W =_{B_O} W +_{A_O} W -_{A_OB_O} W,$$
(5)

where  $_XW = \frac{1}{d_X} \otimes \operatorname{Tr}_X W$ ,  $d_X$  is the dimension of X and  $\operatorname{Tr}_X$  is the partial trace over X.

If a is an input and x is an outcome of the quantum instrument [15], then the quantum instrument can be described by a set of completely positive trace non-increasing maps,  $\{\mathcal{M}_{x|a}^{A}\}_{x}$ , with  $\mathcal{M}_{x|a}^{A}: L(H^{A_{I}}) \to L(H^{A_{O}})$ ,

$$\mathcal{M}_{x|a}^{A}(\sigma) = \sum_{k=1}^{d_{A_{I}}d_{A_{O}}} E_{xk}\sigma E_{xk}^{+}, \text{ for any } \sigma \in L(H^{A_{I}}),$$

where  $E_{xk}: H^{A_I} \to H^{A_O}$  satisfy  $\sum_{k=1}^{d_{A_I}d_{A_O}} E_{xk}^+ E_{xk} \leq \mathbb{1}^{A_I} \quad \forall x, \text{ and } \sum_{x,k} E_{xk}^+ E_{xk} = \mathbb{1}^{A_I}.$ 

As shown in Ref. [3], the assumption of the local quantum framework with no reference to the global causal structure implies that the probability p(x, y|a, b) of two outputs x and y for selecting a pair of Alice and Bob instruments  $(\mathcal{M}_{x|a}^{A})$  and  $\mathcal{M}_{y|b}^{B}$  can be represented by

$$p(x, y|a, b) = \operatorname{Tr}\left[W\left(M_{x|a}^{A_{I}A_{O}} \otimes M_{y|b}^{B_{I}B_{O}}\right)\right],\tag{6}$$

for the process matrix W,  $M_{x|a}^{A_IA_O} = [\mathcal{I} \otimes \mathcal{M}_{x|a}^A (|\varphi^+\rangle \langle \varphi^+|)]^T$  is the Choi matrix [16, 17] of the instrument  $\mathcal{M}_{x|a}^A$ , where  $\mathcal{I}$  is the identity map,  $|\varphi^+\rangle = \sum_{k=1}^{d_{A_I}} |kk\rangle \in H^{A_I} \otimes H^{A_I}$  is the non-normalized maximally entangled state. In this paper, we also call the Choi matrix  $M_{x|a}^{A_IA_O}$  as an instrument. It can be shown that the instruments should satisfy the following conditions [3, 5]:

$$\sum_{x,y} \operatorname{Tr} \left[ W \left( M_{x|a}^{A_{I}A_{O}} \otimes M_{y|b}^{B_{I}B_{O}} \right) \right] = 1,$$

$$\operatorname{Tr}_{A_{O}} \sum_{x} M_{x|a}^{A_{I}A_{O}} = \mathbb{1}^{A_{I}},$$

$$\operatorname{Tr}_{B_{O}} \sum_{y} M_{y|b}^{B_{I}B_{O}} = \mathbb{1}^{B_{I}},$$
(7)

for any  $a, b, M_{x|a}^{A_I A_O}, M_{y|b}^{B_I B_O} \ge 0.$ 

Let  $d_{A_O} = d_{B_O} = 1$ , it is easy to see that the process matrices and the instruments generalize the notions of quantum states and positive operator valued measurements (POVMs) respectively.

It was shown in Refs [3, 4] that there exist joint probabilities which satisfies the constraint (6) such that the above mentioned (causal) inequalities (3) and (4) can be violated. More precisely, if Alice and Bob don't respect a causal order, there is a strategy such that the success probability of the games GYNIC and GYNI can go beyond to the bound which are obtained by using all causal strategies.

#### 3. TWO CAUSAL GAMES

In this section, we will introduce two causal games called "guess your neighbor's parity (GYNP)" and "guess your neighbor's parity by tossing a coin (GYNPC)." For simplicity, we suppose the possible input values a and b of Alice and Bob are  $a = (a_1, a_2)$  and  $b = (b_1, b_2)$ , respectively, where  $a_i, b_i = 0, 1$  (i = 1, 2), and the possible values of outputs x and y are 0 or 1. Thus we will establish two new causal inequalities with 4 inputs and 2 outputs which generalize the inequalities (3) and (4) to the multi-settings.

**GYNP causal game.** Note that the parity of the input  $a = (a_1, a_2), a_1, a_2 \in \{0, 1\}$  is defined by parity $(a) = a_1 + a_2 \pmod{2}$ . In the game GYNP, Alice and Bob receive randomly uniform inputs  $a, b \in \{(0, 0), (0, 1), (1, 0), (1, 1)\}$  from the referee. The task of Alice and Bob is to guess each other's parity of inputs. More precisely, the game is defined by letting

$$\left\{ \begin{array}{l} \pi(a,b) = \frac{1}{16}, \\ V(x,y|a,b) = \delta_{x,parity(b)} \delta_{y,parity(a)}, \end{array} \right. \label{eq:parity}$$

where x, y take values in  $\{0, 1\}$ .

**Proposition 3.1** Using the strategy under the causal order, the success probability of the game GYNP is upper bounded by

$$p_{\text{GYNP}} = p(x = parity(b), y = parity(a)) \le \frac{1}{2},$$
(8)

where the parity(a) and parity(b) is always equal to 0 or 1.

*Proof.* We assume that Alice's operation is earlier than Bob's (i.e.,  $A \leq B$ ), in this case, Bob cannot send signal to Alice, and Alice can only make a random guess for Bob's parity, so

$$p(x = parity(b)) = \frac{1}{2}$$

Hence

$$p(y = parity(a), x = parity(b)) \le \frac{1}{2}.$$

Note that the parity of Alice (resp. Bob) can only be 0 or 1 with equal probability. A similar reason holds for the causal order  $B \leq A$ , and a convex mixture cannot increase the upper bound of the success probability.

**GYNPC causal game.** In the game GYNPC, Alice and Bob receive randomly uniform inputs  $a, b \in \{(0, 0), (0, 1), (1, 0), (1, 1)\}$  from the referee. Additionally, Bob has another bit  $b' \in \{0, 1\}$ . To win the game, Alice need to guess the parity of Bob's inputs correctly if b' = 0, and Bob need to guess the parity of Alice's inputs correctly if b' = 1. More precisely, the game is defined by letting  $\pi(a, b, b') = \frac{1}{32}$  and

$$V(x, y|a, b, b') = \begin{cases} \delta_{x, party(b)}, & \text{if } b' = 0\\ \delta_{y, party(a)}, & \text{if } b' = 1. \end{cases}$$

**Proposition 3.2** Using the causal strategy, the success probability of the game GYNPC is upper bounded by

$$p_{\text{GYNPC}} = \frac{1}{2} p(x = parity(b) \mid b' = 0) + \frac{1}{2} p(y = parity(a) \mid b' = 1) \le \frac{3}{4}.$$
(9)

*Proof.* Similar to the proof of 3.1, assuming that the operation of Bob is strictly before than that of Alice's (i.e.,  $B \leq A$ ), Bob can send signal to Alice. So Alice knows Bob's input b, hence

$$p(x = parity(b) \mid b' = 0) = 1.$$

Because Alice cannot send signal to Bob at this moment, Bob has to randomly guess the parity of Alice's inputs, which leads to

$$p(y = parity(a) \mid b' = 1) = \frac{1}{2}.$$

Hence, the overall success probability  $p_{\text{GYNPC}}$  is no more than  $\frac{3}{4}$ .

#### 4. VIOLATION OF THE TWO NEW CAUSAL INEQUALITIES

Violation of the equalities (8) and (9). Suppose that there is no reference made to any definite causal structure between the operations of the players, and also assume that all players admit the quantum mechanics. We can show that there are appropriate process matrices and instruments to violate the (casual) inequalities (8) and (9).

**Theorem 4.1** The causal inequality (8) can be violated in the framework of process matrix.

*Proof.* Note that  $p(a,b) = \pi(a,b) = \frac{1}{16}$ , then using Bayes' law, the causal inequality (8) implies

$$I := \frac{1}{16} \sum_{a,b} p(x = parity(b), y = parity(a)|a, b) \le \frac{1}{2}.$$
 (10)

Therefore, to derive the violation of the casual inequality (8), proper process matrix and quantum instruments are needed to be constructed such that the inequality (10) can be violated. To this end, we consider the following matrix:

$$W = \frac{1}{16} \left( \mathbb{1}^{\otimes 6} + \frac{1}{\sqrt{2}} \sigma_z^{\otimes 5} \otimes \mathbb{1} + \frac{1}{\sqrt{2}} \sigma_z^{\otimes 2} \otimes \mathbb{1}^{\otimes 2} \otimes \sigma_x^{\otimes 2} \right), \tag{11}$$

where  $\sigma_x$  and  $\sigma_z$  are the standard Pauli matrices, 1 is the identity matrix. It is easy to check that W satisfies equations (5), so it is indeed a process matrix. For simplicity, we denote the inputs [0,0], [0,1], [1,0], [1,1] as 1, 2, 3, 4 respectively, and the instruments performed by Alice and Bob are chosen as follows:

$$M_{0|1}^{A_{I}A_{O}} = (|00\rangle_{A_{I}}\langle 00| + |11\rangle_{A_{I}}\langle 11|) \otimes |0\rangle_{A_{O}}\langle 0| = M_{0|4}^{A_{I}A_{O}},$$

$$M_{1|1}^{A_{I}A_{O}} = (|01\rangle_{A_{I}}\langle 01| + |10\rangle_{A_{I}}\langle 10|) \otimes |0\rangle_{A_{O}}\langle 0| = M_{1|4}^{A_{I}A_{O}},$$

$$M_{1|2}^{A_{I}A_{O}} = (|00\rangle_{A_{I}}\langle 00| + |11\rangle_{A_{I}}\langle 11|) \otimes |0\rangle_{A_{O}}\langle 0| + (|01\rangle_{A_{I}}\langle 01| + |10\rangle_{A_{I}}\langle 10|) \otimes |1\rangle_{A_{O}}\langle 1| = M_{1|3}^{A_{I}A_{O}},$$

$$M_{0|2}^{A_{I}A_{O}} = 0 = M_{0|3}^{A_{I}A_{O}},$$

$$M_{0|1}^{B_{I}B_{O}} = (|00\rangle_{B_{I}}\langle 00| + |10\rangle_{B_{I}}\langle 10|) \otimes |1\rangle_{B_{O}}\langle 1| + (|11\rangle_{B_{I}}\langle 11| + |01\rangle_{B_{I}}\langle 01|) \otimes |0\rangle_{B_{O}}\langle 0|$$

$$+ (|0\rangle_{B_{I}}\langle 0| + |1\rangle_{B_{I}}\langle 1|) \otimes (|0\rangle_{B_{I}}\langle 1| \otimes |1\rangle_{B_{O}}\langle 0| + |1\rangle_{B_{I}}\langle 0| \otimes |0\rangle_{B_{O}}\langle 1|) = M_{0|4}^{B_{I}B_{O}},$$

$$M_{1|2}^{B_{I}B_{O}} = (|00\rangle_{B_{I}}\langle 00| + |11\rangle_{B_{I}}\langle 11|) \otimes |0\rangle_{B_{O}}\langle 0| = M_{1|3}^{B_{I}B_{O}},$$

$$M_{0|2}^{B_{I}B_{O}} = (|01\rangle_{B_{I}}\langle 01| + |10\rangle_{B_{I}}\langle 10|) \otimes |0\rangle_{B_{O}}\langle 0| = M_{0|3}^{B_{I}B_{O}},$$

$$M_{0|2}^{B_{I}B_{O}} = (|01\rangle_{B_{I}}\langle 01| + |10\rangle_{B_{I}}\langle 10|) \otimes |0\rangle_{B_{O}}\langle 0| = M_{0|3}^{B_{I}B_{O}},$$

$$(12)$$

where  $\{|0\rangle, |1\rangle\}$  denotes the eigenbasis of the  $\sigma_z$ . It can be checked that the above operators satisfy conditions (7). Substituting equations (11) and (12) into the LHS of (10), after a simple but length calculation (there are 16 terms left in the LHS of equation (10)) we have

$$I = \frac{10 + 5\sqrt{2}}{32} \approx 0.5335 > 0.5.$$
(13)

**Remark 4.2** We can obtain a slightly larger violation of the causal inequality (8) using the following process matrix:

$$W_{r,s} = \frac{1}{16} \left( \mathbb{1}^{\otimes 6} + r\sigma_z^{\otimes 5} \otimes \mathbb{1} + s\sigma_z^{\otimes 2} \otimes \mathbb{1}^{\otimes 2} \otimes \sigma_x^{\otimes 2} \right),$$
(14)

where r and s are coefficients that satisfy  $r^2 + s^2 \leq 1$ . Using the same instruments (12), substituting equations (12) and (14) into the LHS of (10), then we have

$$p_{\rm GYNP}(r,s) = \frac{5}{16} + \frac{3r+2s}{16}.$$
(15)

By taking the extremum of the above equation in the condition of  $r^2 + s^2 \leq 1$  we have

$$\max_{r,s,r^2+s^2 \le 1} p_{\text{GYNP}}(r,s) = \frac{5+\sqrt{13}}{16} \approx 0.5378 > 0.5335.$$
(16)

**Theorem 4.3** There are a suitable process matrix and quantum instruments such that the causal inequality (9) can be violated.

*Proof.* We will derive a violation of this causal inequality in the framework of process matrix. To this end, we construct the following matrix W:

$$W = \frac{1}{16} \left( \mathbb{1}^{\otimes 6} + \frac{1}{\sqrt{2}} \mathbb{1}^{\otimes 2} \otimes \sigma_z^{\otimes 3} \otimes \mathbb{1} + \frac{1}{\sqrt{2}} \sigma_z^{\otimes 2} \otimes \mathbb{1} \otimes \sigma_z \otimes \sigma_x \otimes \sigma_z \right).$$
(17)

It is easy to check that W is indeed a process matrix. To obtain the violation, Alice and Bob choose the following instruments:

$$M^{A_{I}A_{O}}(x,a) = \frac{1}{4} [\mathbb{1}^{\otimes 2} + (-1)^{x} \sigma_{z}^{\otimes 2}]^{A_{I}} \otimes [\mathbb{1} + (-1)^{parity(a)} \sigma_{z}]^{A_{O}},$$
  

$$M^{B_{I}B_{O}}(y,b,b'=0) = \frac{1}{4} [\mathbb{1}^{\otimes 2} + (-1)^{y} \sigma_{z} \otimes \sigma_{x}]^{B_{I}} \otimes [\mathbb{1} + (-1)^{parity(b)+y} \sigma_{z}]^{B_{O}},$$
  

$$M^{B_{I}B_{O}}(y,b,b'=1) = \frac{1}{2} [\mathbb{1}^{\otimes 2} + (-1)^{y} \sigma_{z}^{\otimes 2}]^{B_{I}} \otimes \rho^{B_{O}},$$
(18)

where  $\rho^{B_O}$  denotes an arbitrarily prepared state as b' = 1. To calculate the success probability, recall that

$$p(y|a, b, b' = 1) = \sum_{x} p(x, y|a, b, b' = 1),$$

After a simple calculation, we have

$$p(y|a, b, b' = 1) = \sum_{x} Tr[W \cdot (M^{A_I A_O}(x, a) \otimes M^{B_I B_O}(y, b, b' = 1))]$$
$$= \frac{1}{2} \left( 1 + (-1)^{(parity(a)+y)} \frac{1}{\sqrt{2}} \right).$$

Hence

$$p(y = parity(a)|b' = 1) = \frac{2 + \sqrt{2}}{4}$$

Similarly, we have

$$p(x = parity(b)|b' = 0) = \frac{2 + \sqrt{2}}{4}$$

Therefore, with the process matrix (17) and instruments (18), the success probability is

$$p_{\rm GYNPC} = \frac{2+\sqrt{2}}{4} \approx 0.8535 > 0.75.$$
 (19)

**Remark 4.4** The above results can be extended to a more general case, i.e., Alice and Bob have  $2^n$  inputs. To obtain the violation, we construct the following process matrix:

$$W_n = \frac{1}{2^{2n}} \left( \mathbb{1}^{\otimes 2n+2} + \frac{1}{\sqrt{2}} \mathbb{1}^{\otimes n} \otimes \sigma_z^{\otimes n+1} \otimes \mathbb{1} + \frac{1}{\sqrt{2}} \sigma_z^{\otimes n} \otimes \mathbb{1} \otimes \sigma_z^{\otimes n-1} \sigma_x \otimes \sigma_z \right).$$
(20)

And the instruments for deriving the violation are chosen as follows:

$$M_{n}^{A_{I}A_{O}}(x,a) = \frac{1}{4} \left[ \mathbb{1}^{\otimes n} + (-1)^{x} \sigma_{z}^{\otimes n} \right]^{A_{I}} \otimes \left[ \mathbb{1} + (-1)^{parity(a)} \sigma_{z} \right]^{A_{O}},$$
  

$$M_{n}^{B_{I}B_{O}}(y,b,b'=0) = \frac{1}{4} \left[ \mathbb{1}^{\otimes n} + (-1)^{y} \sigma_{z}^{\otimes n-1} \sigma_{x} \right]^{B_{I}} \otimes \left[ \mathbb{1} + (-1)^{parity(b)+y} \sigma_{z} \right]^{B_{O}},$$
  

$$M_{n}^{B_{I}B_{O}}(y,b,b'=1) = \frac{1}{2} \left[ \mathbb{1}^{\otimes n} + (-1)^{y} \sigma_{z}^{\otimes n} \right]^{B_{I}} \otimes \rho^{B_{O}},$$
(21)

After a straightforward calculation, the success probability is  $\frac{2+\sqrt{2}}{4}$ .

## Maximal violation of the equality (9).

**Theorem 4.5** The bound  $\frac{2+\sqrt{2}}{4}$  is maximal for the causal inequality (9) when we consider an arbitrary process matrix but restrict the instruments to be binary.

*Proof.* A Hilbert-Schmidt basis of  $L(H^X)$ , with  $X = A_I, A_O, B_I, B_O$  is given by the set of generalized Pauli matrices  $\{\sigma_{\nu}^X\}_{\nu=0}^{d_X^2-1}$ , where  $\sigma_0^X = \mathbb{1}, Tr\sigma_{\mu}^X\sigma_{\nu}^X = d_X\delta_{\mu\nu}$  and  $Tr\sigma_j^X = 0, j = 1, \dots, d_X^2 - 1$ . With this basis, the general bipartite process matrix  $W \in L(H^{A_I} \otimes H^{A_O} \otimes H^{B_I} \otimes H^{B_O})$  can be expressed as follows [3, 6]:

$$W = \frac{1}{d_{A_I} d_{B_I}} (\mathbb{1} + \sigma^{A \preceq B} + \sigma^{B \preceq A} + \sigma^{A \not\preceq \not\equiv B}),$$
  

$$\sigma^{A \preceq B} := \sum_{i,j>0} c_{ij} \sigma_i^{A_O} \sigma_j^{B_I} + \sum_{i,j,k>0} d_{ijk} \sigma_i^{A_I} \sigma_j^{A_O} \sigma_k^{B_I},$$
  

$$\sigma^{B \preceq A} := \sum_{i,j>0} e_{ij} \sigma_i^{A_I} \sigma_j^{B_O} + \sum_{i,j,k>0} f_{ijk} \sigma_i^{A_I} \sigma_j^{B_I} \sigma_k^{B_O},$$
  

$$\sigma^{A \not\preceq \not\equiv B} := \sum_{i>0} v_i \sigma_i^{A_I} + \sum_{i>0} x_i \sigma_i^{B_I} + \sum_{i,j>0} g_{ij} \sigma_i^{A_I} \sigma_j^{B_I},$$
(22)

where  $c_{ij}, d_{ijk}, e_{ij}, f_{ijk}, v_i, x_i, g_{ij}$  are real numbers. Note that we have omitted the identity operators and the tensor product symbols in the expressions above.

To prove our conclusion, the operations are limited to be the binary observables. Herein, we firstly introduce the traceless dichotomic observables, which have two outcomes (eigenvalues), i.e, 1 and -1. Let  $O_{\vec{n}} = \sum_{i>0} n_i \sigma_i^X := (\vec{n} | \vec{\sigma}^X)$  and  $O_{\hat{S}} = \sum_{i,j>0} S_{ij} \sigma_i^X \otimes \sigma_j^X := (\hat{S} | \vec{\sigma}^X \otimes \vec{\sigma}^X)$ , where  $(\cdot | \cdot)$  denotes the inner product in Euclidean space and  $X = A_I, A_O, B_I, B_O$ . Since  $O_{\vec{n}}^2 = \mathbb{1}$  and  $O_{\hat{S}}^2 = \mathbb{1}$ , so  $\|\vec{n}\| = 1$  and  $\|\hat{S}\| = 1$ ,  $\|\cdot\|$  denotes the 2-norm. Similarly, we can define operators  $O_{\vec{n}}, O_{\vec{r}}, O_{\vec{s}}, O_{\vec{t}}$  and  $O_{\hat{T}}$ , where  $\|\vec{m}\| = \|\vec{r}\| = \|\vec{t}\| = \|\vec{s}\| = 1$  and  $\|\hat{T}\| = 1$ . To obtain the violation for the causal inequality (9), the instruments of Alice and Bob are chosen as follows:

$$M^{A_{I}A_{O}}(x,a) = \frac{1}{2d_{A_{O}}} \left( \mathbb{1} + (-1)^{x} (\vec{m} | \vec{\sigma}^{A_{I}}) + (-1)^{F} (\vec{n} | \vec{\sigma}^{A_{O}}) + (-1)^{F \oplus x} (\hat{T} | \vec{\sigma}^{A_{I}} \otimes \vec{\sigma}^{A_{O}}) \right),$$
  

$$M^{B_{I}B_{O}}(y,b,b'=1) = \frac{1}{2} \left( \mathbb{1} + (-1)^{y} (\vec{r} | \vec{\sigma}^{B_{I}}) \otimes \rho^{B_{O}} \right),$$
  

$$M^{B_{I}B_{O}}(y,b,b'=0) = \frac{1}{2d_{B_{O}}} \left( \mathbb{1} + (-1)^{y} (\vec{t} | \vec{\sigma}^{B_{I}}) + (-1)^{G} (\vec{s} | \vec{\sigma}^{B_{O}}) + (-1)^{G \oplus y} (\hat{S} | \vec{\sigma}^{B_{I}} \otimes \vec{\sigma}^{B_{O}}) \right),$$
(23)

where the  $F \in \{0,1\}$  depends on x and parity(a) (resp.  $G \in \{0,1\}$  depends on parity(b) and y), sign  $(-1)^{F \oplus x}(\text{resp.}(-1)^{G \oplus y})$  is set to ensure the complete positivity of the instruments,  $\rho^{B_O}$  represents the prepared state,  $tr\rho^{B_O} = 1$ . Also, the instruments omit the symbol of the identity operators and tensor product on the subsystem space.

By a direct calculation, the possible probabilities for different outcomes are given by

$$p(x = parity(b)|a, b, b' = 0) = \frac{1}{2} \left( 1 + (-1)^{parity(b)}(\vec{v}|\vec{m}) + (\hat{e}|\vec{m} \otimes \vec{s}) \right) or$$

$$p(x = parity(b)|a, b, b' = 0) = \frac{1}{2} \left( 1 + (-1)^{parity(b)}(\vec{v}|\vec{m}) + (\hat{f}|\vec{m} \otimes \hat{S}) \right),$$

$$p(y = parity(a)|a, b, b' = 1) = \frac{1}{2} \left( 1 + (-1)^{parity(a)}(\vec{x}|\vec{r}) + (\hat{e}|\vec{n} \otimes \vec{r}) \right) or$$

$$p(y = parity(a)|a, b, b' = 1) = \frac{1}{2} \left( 1 + (-1)^{parity(a)}(\vec{x}|\vec{r}) + (\hat{d}|\hat{T} \otimes \vec{r}) \right),$$
(24)

where  $\vec{x} = (x_i), \vec{v} = (v_i), \hat{c} = (c_{ij}), \hat{d} = (d_{ijk}), \hat{e} = (e_{ij}), \hat{f} = (f_{ijk})$  are the terms introduced in equations (22). After averaging the first and the second equations over b, as well as the third and the fourth equations over a, and then inserting them in equation (9). The corresponding maximal success probability are obtained as follows:

$$p_{\text{GYNPC}}^{\text{max}} = \max_{\vec{n}, \vec{r}, \vec{m}, \vec{s}} \frac{1}{4} \left( 2 + (\hat{c} | \vec{n} \otimes \vec{r}) + (\hat{e} | \vec{m} \otimes \vec{s}) \right),$$

$$p_{\text{GYNPC}}^{\text{max}} = \max_{\vec{n}, \vec{r}, \vec{m}, \hat{S}} \frac{1}{4} \left( 2 + (\hat{c} | \vec{n} \otimes \vec{r}) + (\hat{f} | \vec{m} \otimes \hat{S}) \right),$$

$$p_{\text{GYNPC}}^{\text{max}} = \max_{\hat{T}, \vec{r}, \vec{m}, \vec{s}} \frac{1}{4} \left( 2 + (\hat{d} | \hat{T} \otimes \vec{r}) + (\hat{e} | \vec{m} \otimes \vec{s}) \right),$$

$$p_{\text{GYNPC}}^{\text{max}} = \max_{\hat{T}, \vec{r}, \vec{m}, \hat{S}} \frac{1}{4} \left( 2 + (\hat{d} | \hat{T} \otimes \vec{r}) + (\hat{f} | \vec{m} \otimes \hat{S}) \right).$$
(25)

Recall that there are three vectors  $\vec{a}, \vec{b}$  and  $\vec{i}$  introduced in Ref. [14]:  $\vec{a} = (\mathbb{1} \otimes O_{\vec{n}} \otimes O_{\vec{r}} \otimes \mathbb{1}) \sqrt{\rho}, \vec{b} = (O_{\vec{m}} \otimes \mathbb{1}^{\otimes 2} \otimes O_{\vec{s}}) \sqrt{\rho},$ and  $\vec{i} = (\mathbb{1}^{\otimes 4}) \sqrt{\rho}$ , where  $\rho$  is the density matrix,  $\rho = \frac{1}{d_{A_O} d_{B_O}} W$ . These vectors satisfy  $(\vec{a}|\vec{a}) = (\vec{b}|\vec{b}) = (\vec{i}|\vec{i}) = 1$  and  $(\vec{a}|\vec{i}) = (\hat{c}|\vec{n} \otimes \vec{r}), (\vec{b}|\vec{i}) = (\hat{e}|\vec{m} \otimes \vec{s}), (\vec{a}|\vec{b}) = 0$ , where the inner product between two vectors  $\vec{a} = A$  and  $\vec{b} = B$  is defined by the inner product of the corresponding matrices:  $(\vec{a}|\vec{b}) := Tr(A^{\dagger}B)$ . Therefore the first equation in (25) (other equations can be treated analogously) can be restated as

$$p_{\text{GYNPC}}^{\text{max}} = \max_{\vec{a},\vec{b}} \frac{1}{4} \left( 2 + (\vec{a}|\vec{i}) + (\vec{b}|\vec{i}) \right) \le \frac{2 + \sqrt{2}}{4}.$$
(26)

### 5. CONCLUSIONS

In this paper, we have extended the causal inequality in Ref. [4] to the 4 inputs case, and the causal inequality in Ref. [3] to the  $2^n$  inputs case. The original inequalities (3) and (4) can be explained by the causal games "guess your neighbor's inputs by tossing a coin" and "guess your neighbor's inputs " respectively. And there are 2 inputs for Alice and Bob in those games. Instead of guessing the inputs, our games consider the success of guessing the parity of the inputs. Our new causal inequalities can be violated in the framework of process matrix. Noticeably, the causal inequality (8) obtained above can also be extend to  $2^n$  inputs case, it is direct but lengthy. Moreover, for the inequality (9), our violation is maximal in the sense of restricting the instruments to be binary ones.

We concludes our paper with the following two questions: Is it possible to extend the multipartite causal inequalities considered in Ref. [11] and Ref. [12] to the multi-settings? Is it possible to derive a dimension witness in terms of causal inequality, i.e., to find a causal inequality whose upper bound in the framework of process matrix only depends on the dimension.

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